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Electronic Structure of Heteroepitaxial Copper Phthalocyanine on Au(001)

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Beamline(s): U4A

Introduction: Understanding of the initial growth structures of metallophthalocyanine films is important for the design of potential molecular devices. Careful studies of these films grown into highly ordered structures can bring a new understanding of interfacial chemistry and physics involving metallophthalocyanines. In order to determine the nature of bonding, orbitals, and geometry between CuPc and Au at the initial growth stage, the soft x-ray photoemission experiments were conducted in the ultra-high vacuum chamber at the NSLS U4A beamline.

Methods and Materials: The Au(001) surface was treated with the standard preparation methods of several cycles of Ar ion sputtering and low temperature annealing (T < 250 °C), resulting in the well-known "5x20" low energy electron diffraction (LEED) pattern. CuPc was evaporated onto the reconstructed Au surface by resistively heating a BN crucible of CuPc powder in the UHV chamber at T < 317 °C. The commercially available CuPc powder was used without further purification except for repeated degassing of the source prior to the actual experiment.

Results: The deposited CuPc overlayer resulted in a new "1x1" LEED pattern (Fig. 1). The surface unit mesh vectors of the CuPc LEED coincide with the <110> and $<1\bar{1}0>$ of Au(001) within the experimental error. The surface unit cell of the heteroepitaxial CuPc is estimated as 12.7 Å by 12.7 Å. The value of 12.7Å suggests that the CuPc overlayer is likely incommensurate but with the definite rotational registry to the substrate. The valence band (VB) spectra of CuPc/Au(001) were taken with two different photon energies hν = 27 eV and 125 eV (Fig. 2). At hν = 27 eV, the photoionization cross sections for the carbon, nitrogen, and copper valence orbtials are all comparable in magnitude whereas at hν =125 eV, the Cu *d* orbtials have much larger cross sections than the rest of the valence orbitals of CuPc. Consequently, the VB spectra with the photon energy of 125 eV provide a view, "enhanced" with the Cu *d* characters. The first three major VB peaks at 1.40 eV, 3.55 eV, and 5.80 eV from the Fermi level in the hν =125 eV photoemission spectrum are compared well to the calculated ionization potentials of 0.95 eV ($11b_{2g}$), 2.81 eV ($13a_{1g}$), 3.26 eV ($4e_g$), 4.51 eV ($8b_{1g}$), and 5.35 eV($12a_{1g}$) for the molecular orbitals with significant *d* characters.

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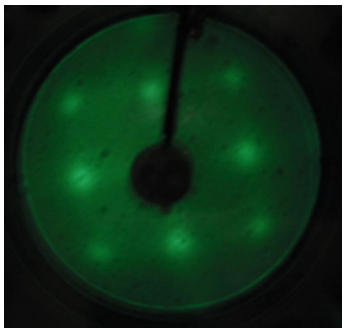

Fig. 1 LEED from 14 Å CuPc/Au(001) at E = 13.4 eV

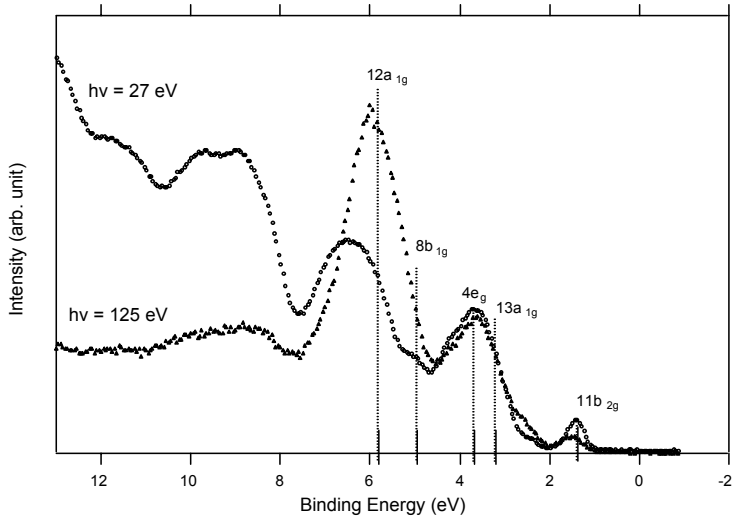

Fig. 2 The VB spectra from 27 Å CuPc/Au(001)